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Friction stress effects on mode I crack growth predictions

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Abstract

The effect of a lattice friction stress on the monotonic growth of a plane strain mode I crack under small-scale yielding conditions is analyzed using discrete dislocation plasticity. When the friction stress is increased from zero to half the dislocation nucleation stress, the crack tip stress field changes from one characteristic of a plastic solid to one characteristic of an elastic solid, and the crack growth resistance decreases substantially.

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Keywords: Dislocation; Theory; Fracture; Micromechanical modeling

1. Introduction

Quite generally, a dislocation is mobile only if a finite stress acts on it. One source of the inherent resistance to motion is the Peierls–Nabarro stress [1,2] which arises as a consequence of the discreteness of an atomic lattice. The ratio of the Peierls–Nabarro stress τ_f to the elastic shear modulus μ has a sensitive dependence on crystal structure. For example, at 0 K, $\tau_f/\mu \approx 10^{-6}$ and 10^{-3} for fcc and bcc metals, respectively, while it is significantly larger ($\tau_f/\mu \approx 10^{-1}$) for many intermetallics [3]. These values are strongly affected by temperature, with τ_f/μ reducing at room temperature to as little as 20% of its value at 0 K for bcc metals such as Nb and α -Fe as noted in [4]. Inter-

actions with solutes can also trap dislocations and give rise to a resistance to dislocation motion that, phenomenologically, is like that associated with the Peierls–Nabarro stress [5]. We refer to any such barrier to dislocation motion as a friction stress.

The Peierls–Nabarro stress plays an important role in governing the brittle to ductile transition [6]. For example, increasing the Ti alloying content in Nb-based intermetallics increases the fracture toughness and this is attributed to a reduction in the lattice Peierls–Nabarro stress of the Nb solid solution phase [7]. Here, the dependence of crack growth behavior on friction stress is investigated via a discrete dislocation plasticity framework in which plastic flow arises from the collective motion of large numbers of dislocations and the fracture properties are embedded in a cohesive surface constitutive relation. In Cleveringa et al. [8] dislocation plasticity based analyses of crack growth were carried out with the friction stress neglected.

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Two limiting cases were found. One is when few dislocations are generated and the crack propagates in a brittle manner. The other is when extensive dislocation activity precedes fracture, with the dislocations substantially relaxing the stresses near the crack tip, leading to continued blunting with a cleavage-type fracture precluded. In the intermediate regime, a cleavage-type fracture occurs in the presence of plasticity with the character of the crack growth resistance response depending on the plastic flow properties. The focus in the present study is on the role of the friction stress in this fracture mode transition.

2. Problem formulation

The boundary value problem, sketched in Fig. 1, is the same as in [8] (also see [9]) where further details can be found. A plane strain region of dimension $L = 1000 \mu\text{m}$ and $h = 500 \mu\text{m}$ is analyzed. Small-scale yielding conditions are assumed and monotonically increasing displacements associated with the mode I elastic singular crack tip field are prescribed. Plastic deformation near the crack tip by the motion of discrete dislocations is accounted for in a process window of dimensions $L_p = 15 \mu\text{m}$ by $h_p = 15 \mu\text{m}$. The calculations were carried out for a crystal with three slip systems having their slip planes oriented at $\theta = \pm 60^\circ$ and $\theta = 0^\circ$ from

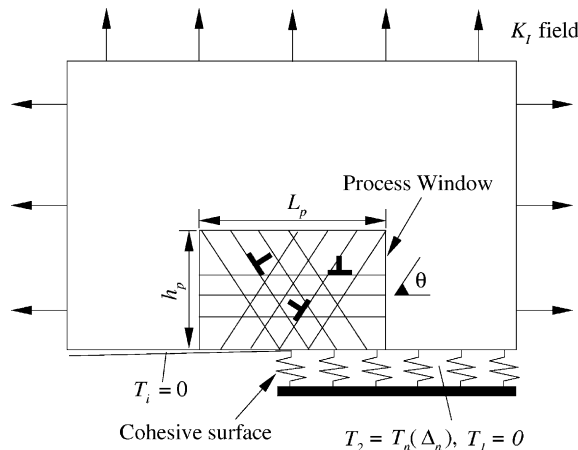


Fig. 1. Sketch illustrating the small-scale yielding boundary value problem.

the crack line. The active slip plane spacing is 100 Burgers vectors. The dislocations are modeled as singularities in a single crystal with isotropic elastic properties specified by the shear modulus $\mu = 26.3 \text{ GPa}$ and Poisson's ratio $\nu = 0.33$. Plastic deformation is assumed to occur by the motion of edge dislocations only, with Burgers vector magnitude $b = 0.25 \text{ nm}$. There is neither cross slip nor climb so that dislocations remain on their slip planes. The glide component of the Peach–Koehler force on dislocation I , $f^{(I)}$, is given by

$$f^{(I)} = b_i \left(\hat{\sigma}_{ij} + \sum_{J \neq I} \tilde{\sigma}_{ij}^{(J)} \right) m_j^{(I)}, \quad (1)$$

where b_i is the Burgers vector, $m_j^{(I)}$ is the slip plane normal, $\tilde{\sigma}_{ij}^{(J)}$ are the interaction stresses with the other dislocations and $\hat{\sigma}_{ij}$ are the image stresses that are due to the boundary conditions.

The magnitude of the glide velocity $v^{(I)}$ of dislocation I is taken to be related to the Peach–Koehler force via

$$v^{(I)} = \begin{cases} (f^{(I)} - b\tau_f \text{sign}(f^{(I)}))/B & \text{if } |f^{(I)}| > b\tau_f; \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

with $B = 10^{-4} \text{ Pa s}$.

The crystal has a random distribution of dislocation sources and point obstacles. The randomly distributed sources with a density of $66/\mu\text{m}^2$ mimic Frank–Read sources from pinned segments on out-of-plane slip systems and generate a dislocation dipole when the magnitude of the Peach–Koehler force exceeds a critical value of $b\tau_{\text{nuc}}$ during a period of time t_{nuc} , with $\tau_{\text{nuc}} = 50 \text{ MPa}$ and $t_{\text{nuc}} = 10 \text{ ns}$. For plane strain tension, with no crack, the uniaxial yield strength is $\approx \tau_{\text{nuc}}$ [10]. The process window also contains a random distribution of 170 point obstacles per μm^2 (which represent either small precipitates on the slip plane or forest dislocations on out-of-plane slip systems) that pin dislocations and release them once the Peach–Koehler force attains $b\tau_{\text{obs}}$, where $\tau_{\text{obs}} = 150 \text{ MPa}$. The values of source and obstacle densities chosen here are higher than dislocation densities corresponding to the Frank network in well-annealed crystals but are considered representative for single crystals that have undergone

small amounts of cold-working [11]. Annihilation of two dislocations on the same slip plane with opposite Burgers vectors occurs when they approach each other within a critical distance $L_c = 6b$.

A cohesive surface is specified ahead of the initial crack tip with cohesive strength $\sigma_{\max} = 0.5$ GPa and work of separation $\phi_n = 1.019$ J/m² (the surface energy of a wide variety of materials is ≈ 1 J/m², see e.g. [12]). This gives a reference stress intensity factor $K_0 = \sqrt{E\phi_n/(1-\nu^2)} \approx 0.28$ MPa $\sqrt{\text{m}}$ at which crack growth would occur in a homogeneous elastic solid with the given cohesive properties.

3. Numerical results

Curves of crack extension, Δa , versus the normalized applied stress intensity factor K_I/K_0 are shown in Fig. 2 for friction stress values $\tau_f/\tau_{\text{nuc}} = 0.25, 0.4$ and 0.5 which, with τ_{nuc} identified with flow strength, are representative of Nb-based intermetallics with varying amounts of Ti alloying [7]. For comparison purposes, a curve for $\tau_f = 0$ is also included. With $\tau_f = 0$, crack growth initiates at $K_I/K_0 \approx 1.4$, and the resistance to crack

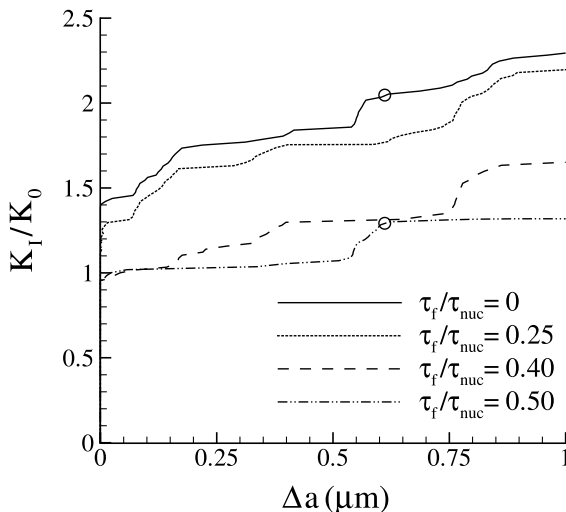


Fig. 2. The applied stress intensity factor K_I/K_0 as a function of crack extension Δa for four values of the friction stress τ_f .

growth rises rapidly as the crack propagates. With $\tau_f \neq 0$, the restricted mobility of dislocations promotes the initiation of crack growth at lower values of the applied K_I/K_0 ; K_I/K_0 at crack initiation is 0.95 for $\tau_f/\tau_{\text{nuc}} = 0.5$ and in this case crack growth proceeds in “spurts” of ≈ 0.5 μm . Similar spurt-like crack growth occurs with the other nonzero values of friction stress, but with the length of the spurts shortened as τ_f is decreased.

A typical characteristic of crack growth in a ductile material is the increase in applied stress intensity factor accompanying crack growth, i.e. a positive $\Delta K_I/\Delta a$. In Fig. 2 there is a transition from a ductile to a brittle type of crack growth behavior between $\tau_f/\tau_{\text{nuc}} = 0.25$ and $\tau_f/\tau_{\text{nuc}} = 0.5$. Experimental measurements of the fracture toughness of Nb-based intermetallics show that the fracture toughness of these alloys is increased by about a factor of two when the Ti alloying is increased to 40% (see [3] and references therein). This is attributed to a reduction in the Peierls–Nabarro lattice stress of the Nb solid solution phase and our numerical results are consistent with these experimental observations.

The crack growth behavior in the computations in Fig. 2 is mainly controlled by a relatively small number of dislocations very near the crack tip. For low values of the friction stress, dislocation glide occurs rather easily and the dislocations nucleated in the near crack tip region either glide away from the crack tip into the material or exit from the crack flanks. This dislocation motion relaxes the near tip stresses and gives rise to crack tip blunting which results in a ductile response. On the other hand, when the friction stress is high, dislocation motion is inhibited and fracture occurs with much less plastic dissipation leading to brittle fracture behavior.

The effect of the friction stress on the near tip dislocation structure and the distribution of the opening stress σ_{22} is illustrated in Fig. 3 for a crack extension $\Delta a = 0.61$ μm . The points corresponding to these states are shown by circles in Fig. 2. With $\tau_f = 0$, Fig. 3a, the near tip stress field, on average, has a form resembling the nonhardening crystal plasticity field of Rice [13]. In contrast, with $\tau_f/\tau_{\text{nuc}} = 0.5$, Fig. 3b, the stress field, except for perturbations associated with individual

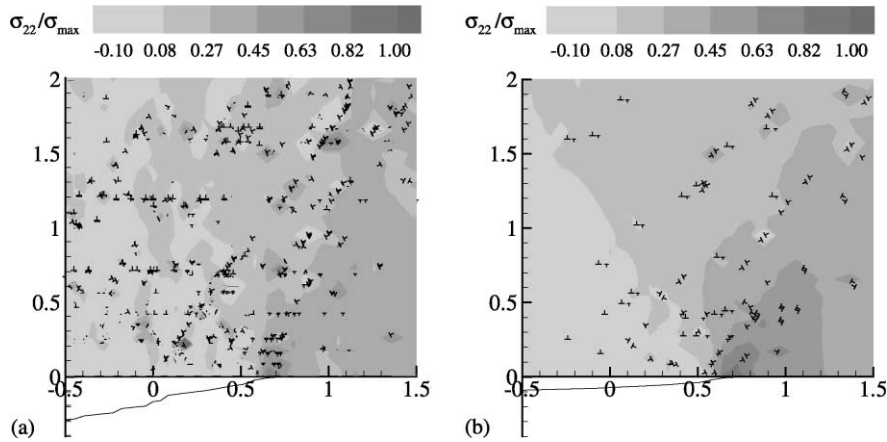


Fig. 3. Distribution of dislocations and the opening stress σ_{22} in the immediate neighborhood ($2 \mu\text{m} \times 2 \mu\text{m}$) of the crack tip for friction stress values $\tau_f/\tau_{\text{nuc}} = 0$ (a) and 0.5 (b) at $\Delta a = 0.61 \mu\text{m}$. The corresponding crack tip profiles (magnified by a factor of 10) are plotted below the x -axis. Distances are in μm .

dislocations, resembles the elastic mode I singular crack tip field.

Fig. 4 shows the dislocation structure and crack opening stress σ_{22} distribution near the crack tip for $\tau_f/\tau_{\text{nuc}} = 0.5$ at two stages of crack growth. At the initiation of crack growth, very few dislocation sources are activated. As K_I/K_0 increases, dislocation activity increases, but with limited dislocation mobility the stress field still closely resembles a mode I elastic field. Fig. 5 shows the

dislocation density (the number of dislocations per unit area of the process window) as a function of the crack extension Δa for the considered values of τ_f . The dislocation density increases with crack extension for low values of τ_f , while the dislocation density is much reduced for $\tau_f/\tau_{\text{nuc}} \geq 0.4$. Due to the decreased dislocation mobility for the higher values of τ_f , dislocation dipoles remain near the source from which they were nucleated. The back stress from these dipoles then tends to inhibit

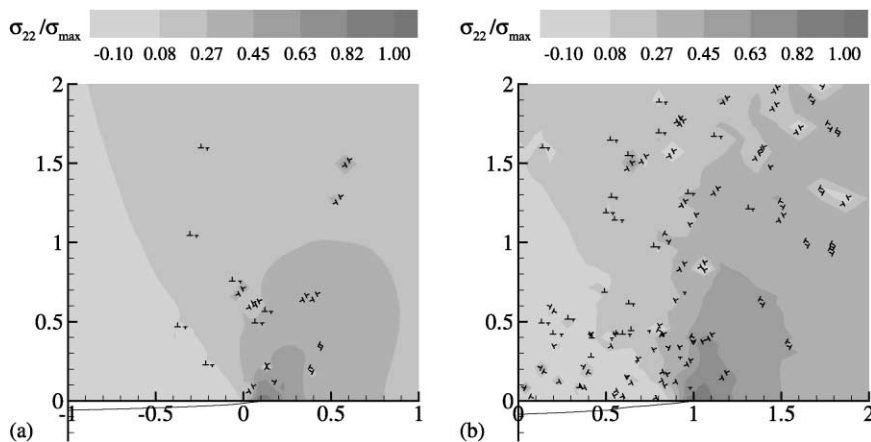


Fig. 4. Distribution of dislocations and the opening stress σ_{22} in the immediate neighborhood ($2 \mu\text{m} \times 2 \mu\text{m}$) of the crack tip for a friction stress $\tau_f/\tau_{\text{nuc}} = 0.5$ at (a) crack growth initiation; and (b) crack extension $\Delta a \approx 1 \mu\text{m}$. The corresponding crack tip profiles (magnified by a factor of 10) are plotted below the x -axis. Distances are in μm .

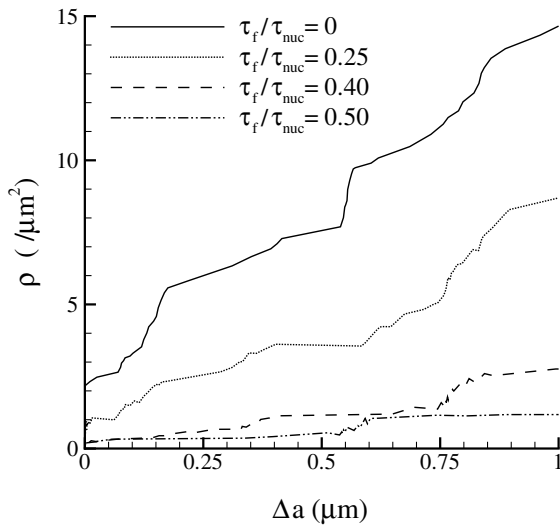


Fig. 5. The dislocation density ρ as a function of crack extension Δa for four values of the friction stress τ_f .

further nucleation. The reduced dislocation glide, of course, also means that there is much less plastic dissipation.

4. Conclusions

We have carried out analyses of the growth of a plane strain mode I crack under monotonic small-scale yielding conditions for single crystals having various values of the friction stress. The fracture properties of the material are embedded in a cohesive surface constitutive relation and plastic flow arises from the collective motion of a large number of discrete dislocations.

With increasing friction stress, from zero to $0.5\tau_{\text{nuc}}$ in the calculations here, the mobility of dislocations is reduced and the stress level in front

of the crack tip increases significantly due to the presence of stationary dislocations. The near crack tip stress field changes from one characteristic of a plastic solid to one resembling that of an elastic solid. As a consequence, with increasing friction stress, crack initiation occurs at a lower value of the applied K_I and the crack growth resistance, as measured by the average slope $\Delta K_I/\Delta a$, decreases.

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